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The 7s Excited State of the Cesium Atom

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Abstract

A technique has been developed for the calculation of excited state, one-electron wave functions based on the Thomas-Fermi statistical theory of the atom. The technique is applicable to heavy atoms for which Hartree type solutions are complex and difficult to obtain. In this paper the previously obtained Thomas-Fermi core potential for the cesium atom and a Heisenberg type polarization correction is used as a central field in the Schrödinger equation. Correction for penetration of the excited electron's orbital is made, and the Biermann-Lübeck approach for solving the wave equation is utilized. This allows for the inclusion of a qualitative correction for exchange. The cesium atom's 7s excited state which has not been obtained by any Hartree method is computed.

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1. Introduction.

The only systematic approach to the calculation of atomic structure and properties is via the Hartree [1] or Hartree-Fock [2] approximation. However, there are limitations to these calculations. Their numerical complexity makes it difficult to obtain an overall physical picture of the atom. Only isolated solutions are possible in these approximations and for heavy atoms the numerical complexity of the self consistent iterations makes the calculations for atomic structure all but impossible.

There are additional complications which arise when attempting to calculate the structure of excited states since one requires that the wave functions used be orthogonal to all lower states, and it is sometimes impossible to obtain solutions with this requirement.

For those states for which Hartree or Hartree-Fock one-electron wave functions cannot be obtained, one can use a somewhat cruder approximation which has the advantage of simplicity, namely the Thomas-Fermi model [3,4]. The basic assumptions in this model, however, require that we investigate only the ground state configurations. Some attempts have been made by Latter [5] to investigate the excited states of an electron in the Thomas-Fermi central potential. This is of course an approximation to the description of excited states of atoms since, for example, some self-force on the electron is included and there is no correction for interaction effects. A procedure has been previously described by this author [6,7] which is a combination of the Thomas-Fermi technique and a self-consistent procedure. It is easiest to apply in cases where there are several closed shells and the excitations being discussed are those of electrons outside these closed shells. The excited electron is considered to move in the Thomas-Fermi field of the remaining electrons, and a self-consistent procedure is used to account for the distortion

of the Thomas-Fermi field due to the penetration of the charge cloud by the excited electron. In this report, the solution to the 7s excited state of the cesium atom is presented.

2. The General Technique.

For an alkali atom, we first neglect the interaction of the excited electron with the remaining ion core. The ion core can then be treated by the Thomas-Fermi technique since the remaining core electrons are all in the ground state, and for a heavy ion, well approximated by a continuous distribution. Such an ionic system obeys the following differential system [8]

$$\phi''(x) = \phi^{3/2}(x)/x^{1/2} \tag{2.1}$$

with $\phi(0) = 1,$ (2.2)

$$\phi(x_o) = 0, \tag{2.3}$$

$$x_o\phi'(x_o) = -(Z-N)/Z \tag{2.4}$$

where $\phi(r) = r\left[V(r)-V_o\right]/Ze$ (2.5)

$$x = r/a_o(9\pi^2/128Z)^{1/3} = rZ^{1/3}/0.885341a_o \tag{2.6}$$

with $V(r)$, the radially symmetric potential; a_o, the first Bohr radius; Z, the nuclear charge; N, the number of electrons in the ion core; and r_o, the effective radius of the ion, being defined such that for $r>r_o$, $V(r) = (Z-N)e/r$.

Solving this set of equations yields a potential distribution for the core which will be called $V_{\text{ion core}}$. The solution of the Thomas-Fermi ion has been given in reference [6].

The potential will not be exactly the ion that the excited electron moves in. Even for a completely non-penetrating outer electron, which might be expected to move in a completely hydrogen-like Coulomb field, there is produced a resultant asymmetry or polarization which leads to slightly greater binding energy for the nonpenetrating electron than for the hydrogenic electron. In the present analysis

this correction is made using a term introduced by Born and Heisenberg [9], the argument being presented in reference [7]. The latter shows there exists a polarization energy of

$$U_{pol} = -\alpha_p e^2/2r^4 , \tag{2.7}$$

where α_p is the polarizability of the ion core. Its value for the cesium ion is approximately 2.42 in 10^{-24} units.

3. Solution of the Schrödinger Equation.

The charge distribution and consequently the potential of the ion can now be used as a central field in which the valence electron moves. The calculated excited and/or ground state one-electron wave functions will give the charge distribution of the valence electron for the states considered. This statement is only approximately true for several reasons, the most important of which is that we have calculated a charge distribution for the core which is good only in the Thomas-Fermi approximation. Other approximations which will have to be made concern the partial shielding of the core due to the penetration of the valence electron's charge distribution, the exchange effects, and the dynamical aspects of the problem which include the deformation of the core due to the presence of the penetrating electron. It will be seen that these last three effects can be included approximately in our calculation.

If we consider a separable, product type wave function, and make the further assumption that angular dependence can be separated out, the one-electron wave function of the i^{th} electron is given by

$$\psi_i = R(r)Y_{\ell,m}(\theta,\phi) = [X(r)/r]Y_{\ell,m}(\theta,\phi) \tag{3.1}$$

and the wave equation for the valence electron moving in the field of the Thomas-Fermi potential of the ion is

$$X_i''(r) - \left[(2m\epsilon_i/\hbar^2) - (2meV_{TF}(r)/\hbar^2) + (\ell)(\ell+1)/r^2\right] X_i(r) = 0 \qquad (3.2)$$

where $Y_{\ell,m}(\theta,\phi)$ are the spherical harmonic functions, $V_{TF}(r)$ the core potential, ℓ the angular momentum quantum number, and ϵ_i the corresponding eigenvalue. In accordance with normalization we further require that

$$\int_0^\infty r^2 R(r)R^*(r)dr = \int_0^\infty X(r)X^*(r)dr = 1. \qquad (3.3)$$

It is seen from the above that after angular dependence is separated out, the remaining second-order equation can be put into a form that does not contain the first derivative by introducing the $X(r)$ function. It is then amenable to numerical integration by the Milne [10] method or by standard numerical techniques due to Hartree [11], Gauss-Jackson-Jumerov [12,13], and Blanch [14].

As indicated in Section 2, the Heisenberg form for the polarization potential energy is $-\alpha_p e^2/2r^4$, where the argument for its determination holds only in the region outside the core. If this term were added only in the outer region, there would be a discontinuity at the core boundary. Following Biermann and Harting [15] we add a polarization term of the form $(\alpha_p e^2/2r^4)\left[1-e^{-(r/fr_o)^8}\right]$ for the inner region as well. Here f is a fraction which was taken as 0.4 for this calculation. Although the exponent can be raised to any power greater than four, eight was found to give the best fit with optical values [15]. The addition of this term has the effect of eliminating the polarization term in the core until $r = fr_o$. It then goes smoothly into the $1/r^4$ behavior at the core boundary. Although strictly speaking this is an empirical correction it is a small one, and too much concern need not be given to the exact form of the correction.

A useful apporach to the solution of the wave equation is that developed by Biermann and Lübeck [16]. In addition to the polarization contribution, and

being adaptable to the Thomas-Fermi potential, the method also allows for the inclusion of a semi-empirical exchange correction. Introduction of the latter correction has the effect of introducing a non-experimentally determined parameter into a system which is already determined without redundancy. In order to compensate for this while calculating the best possible wave function for the assumed potential (originally taken as the Hartree potential), Biermann and Lübeck solve the wave equation utilizing the experimentally determined term value. Accurate listings of these values can presently be found in Circular 467 of the National Bureau of Standards [17]. Starting with this experimental term value is not necessarily an unfair approach since both Hartree and Thomas-Fermi potentials do lead to term values which are very close to the experimentally determined ones.

The exchange correction made by Biermann and Lübeck can be applied here by multiplying the Thomas-Fermi central potential distribution by the function

$$B(r) = (1 + \beta r e^{-(r/fr_o)^8}) \quad ; \tag{3.4}$$

for the computation it is convenient to express r and β coefficients of the exponential in $\mathring{A}$ and $1/\mathring{A}$ units, respectively. With this approach the radial wave equation to be solved is now

$$\chi'' - \left[\frac{2m\epsilon_{exp}}{\hbar^2} - \frac{2m\epsilon V(r)}{\hbar^2} + \frac{(\ell)(\ell+1)}{r^2} - \frac{\alpha_{pe}^2}{2r^4}\left(1-e^{-(r/fr_o)^8}\right)\right]\chi = 0 \tag{3.5}$$

where $$V(r) = \left[Ze\phi(r)/r - e/r_o\right]\left[1+\beta r e^{-(r/fr_o)^8}\right] = 0 \; ; \quad 0 \leq r \leq r_o \tag{3.6}$$

and $$V(r) = (e/r)\left[1+\beta r e^{-(r/fr_o)^8}\right] \; ; \quad r > r_o \; . \tag{3.7}$$

The solution of the equation for large values of r is given as $\chi(r) = ke^{\pm\sqrt{2m\epsilon_i}\,r/\hbar}$. Varying β for a particular eigenvalue and angular momentum state leads to solutions such that all diverge as $^{\pm}e^{+ar}$ except the one associated with the desired value of β; in this case we have the physically required exponential decay.

Since this procedure takes advantage of the experimentally determined term value, and makes at least partial correction for almost all other effects, it can be expected to yield fairly accurate wave functions, even for excited states. Indeed this is the case and Biermann and Lübeck find that oscillator strengths for the states in the principal series agree very well with those obtained from experimental measurements. The Biermann and Lübeck procedure neglects, however, the effect of the penetration of the excited electron into the core, and the modification of the core potential due to this penetration. While this is a small correction in the case of the more highly excited levels, it can be significant for the first few excited states. It is possible to include the effect of this penetration by utilizing a self consistent iterative process described in reference [7], and summarized in the next section.

4. The Self Consistent Technique.

The effect of the penetration of the valence electron into the core is partially to shield the nuclear charge and consequently to increase the size of the ion core. The form of the core charge distribution also changes, and with it, the effective potential in which the valence electron moves changes. Since the effective potential depends on the charge distribution, and this in turn depends on the effective potential, we have in principle the ingredients of a self consistent procedure.

We first solve the problem neglecting penetration of the core. If the portion of the computed excited electron's charge distribution penetrating the core is α,

the core size increases somewhat, and the potential at the edge of the core becomes $(Z-N-\alpha)e/r_o'$, where r_o' is the new core radius. This new core potential combined with the polarization contribution is used to solve the Schrödinger equation for the new charge distribution until the solution is self consistent.

There are complications in carrying out this procedure. The penetration not only leads to a modified set of boundary conditions, but strictly speaking, to a modified Thomas-Fermi equation as well.

The Thomas-Fermi potential distribution for the pure ion represents a zeroth order approximation to the ion core. We can use this potential with a polarization correction in the Schrödinger equation to calculate an energy eigenvalue and a wave function for the excited electron e^* which is in some state characterized by specific principal and azimuthal quantum numbers. From the one electron wave function, ψ_{e^*}, so determined, we can calculate a number density for the excited electron

$$n_{e^*} = \left|\psi_{e^*}\right|^2 . \tag{4.1}$$

We can also define a dimensionless potential, that is calculated from the potential V_{e^*} as determined by Poisson's equation, $\nabla^2 V_{e^*} = 4\pi\, n_{e^*} e$:

$$\phi_{e^*} = rV_{e^*}(r)/Ze. \tag{4.2}$$

It is shown in reference [7], that if this potential is taken into account, the core potential, ϕ_{TF}, must now satisfy a modified Thomas-Fermi equation,

$$\phi''_{TF}(x) - \phi''_{e^*}(x) = \phi_{TF}^{3/2}(x)/x^{1/2} . \tag{4.3}$$

As in the case for the pure ion, the boundary conditions at the nucleus and limit-

ing radius are

$$\phi_{TF}(x) = 1 \quad ; \quad \phi_{TF}(x_o) = 0. \tag{4.4}$$

The detail, but not the physical content, of the third boundary relation alters. It becomes

$$-(Z-N-\alpha)/Z = x_o \phi'_{TF}(x_o) \quad . \tag{4.5}$$

5. Starting Values.

The inner region starting values can be obtained by expanding $X(r)$ as a power series in r, substituting into the differential equation and setting the collected coefficients of the r powers to zero. If exchange effect near the origin is neglected, we can write the Schrödinger equation as

$$X''(r) - \left[\sigma + s_1/r^2 - s_2\phi(r)/r\right]X(r) = 0 \tag{5.1}$$

where

$$\sigma = 2m/\hbar^2(\epsilon - eV_o) \quad , \; s_1 = (\ell)(\ell+1) \quad , \text{ and } s_2 = 2me^2Z/\hbar^2. \tag{5.2}$$

Expressing the wave function in power series form

$$X(r) = \sum_{n=0}^{\infty} a_n rn \quad , \tag{5.3}$$

and the collected coefficient of the general term r^m is

$$(m+1)(m+2)a_{m-2} - \sigma a_m + s_2\phi(r)a_{m-1} - s_1 a_{m-2} = 0 \; . \tag{5.4}$$

The $\phi(r)$ function varies between zero and unity through the entire inner region and is treated as a parameter in the expansion. The series must be evaluated from

m = -2 since there is an inverse square term. Combining the above results for the various angular momenta yields the following expansion for the s state:

$$\chi_{s\text{-state}}(r) = a_1\Big[r - (s_2\phi(r)/2)r^2 + (1/6)\Big[(\sigma + s_2^2\phi^2(r)/2)\Big]r^3$$
$$-(1/12)(s_2\phi(r)/2)\Big[\sigma + (1/3)(\sigma + s_2^2\phi^2(r)/2)\Big]r^4$$
$$+(1/20)\Big\{(\sigma/6)(\sigma + s_2^2\phi^2(r)/2)$$
$$- s_2^2\phi^2(r)/(24)\Big[\sigma - (1/3)(\sigma + s_2^2\phi^2(r)/2)\Big]\Big\}r^5 \quad . \; . \; .\Big] \tag{5.5}$$

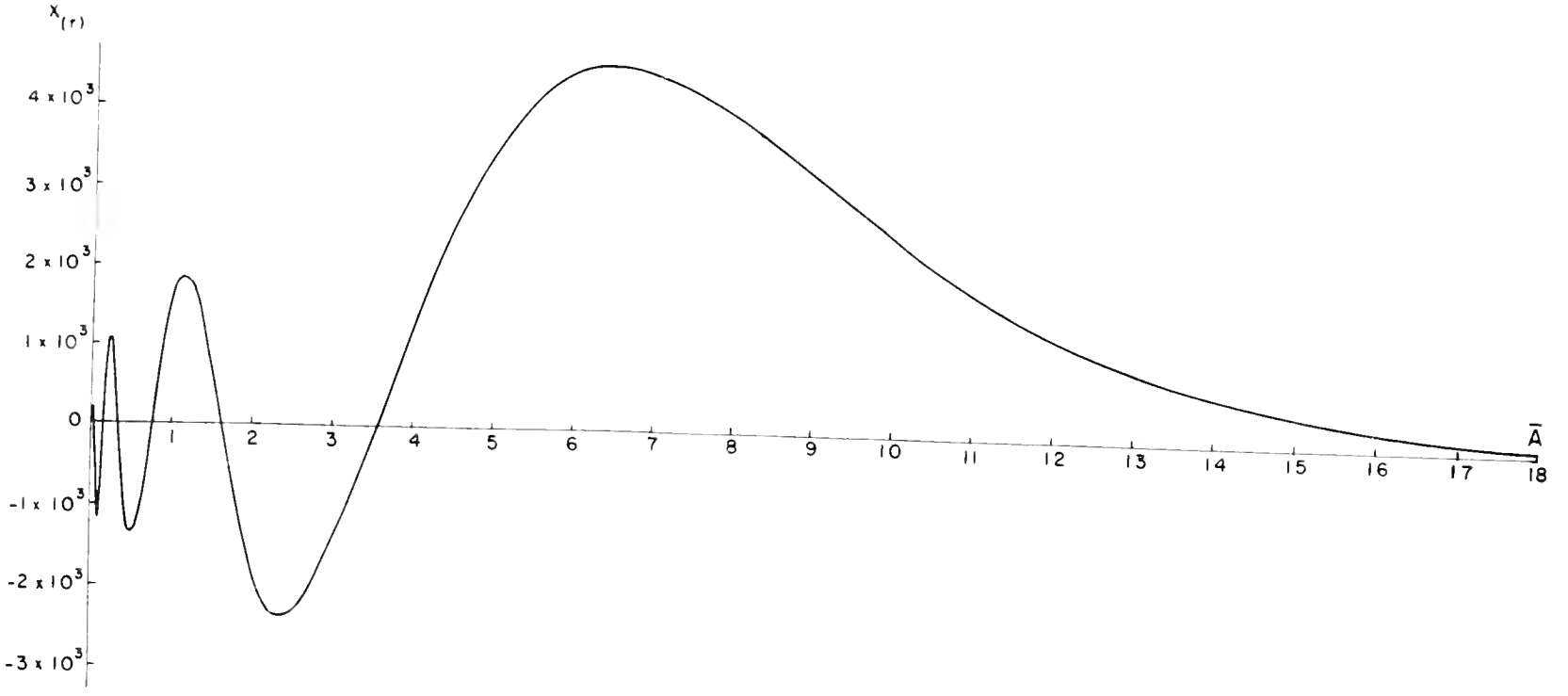
Even neglecting the exchange correction term, the coefficients are seen to become complex as higher powers are needed. Unfortunately it will be seen that heavy atom wave functions are rapidly changing in the strong Coulomb field near the nucleus, and even if a fairly small interval is taken for the $\chi(r)$ tabulation, using the Milne method of integration, the starting value calculation becomes tedious. Although the present calculation was carried out in this manner, the authors recommend the Gauss-Jackson-Numerov [12,13] method for future work. In that case, only two or three terms in the expansion in (5.5) are needed. The approach requires that the Thomas-Fermi potential be determined at irregular intervals near the origin, but that is less cumbersome than determining the starting values using a fifth or sixth degree polynomial.

It can also now be pointed out that the parameter in the Biermann and Lübeck scheme must be known with ever greater accuracy as heavier atoms are studied. In their original work, Biermann and Lübeck required only three significant figures for convergence. D. Villars [18] noted that five figures were required for his work

with potassium. Unfortunately, for the 55 electron cesium atom, eight significant figures were found to be necessary. This begins to exhaust the capabilities of even advanced computers, and the author suggests that for heavier atoms, the Ridley [19] scheme be used since the exchange correction is smaller.

6. Results.

As discussed, the 7s state of the relatively heavy cesium atom was calculated using the above procedure. This state is only one excited level above the ground state and therefore shows a fair degree of penetration. Using the Biermann and Lübeck computing approach, with the experimental term value of 2.556439×10^{-12} ergs, a final degree of penetration, α, was determined as 7.07%. Figure 1 presents the determined wave function, Figure 2 shows the inner region expanded, and Figure 3 illustrates the probability distribution. Table 1 presents a summary, and Table 2 presents the full detail of the calculation.

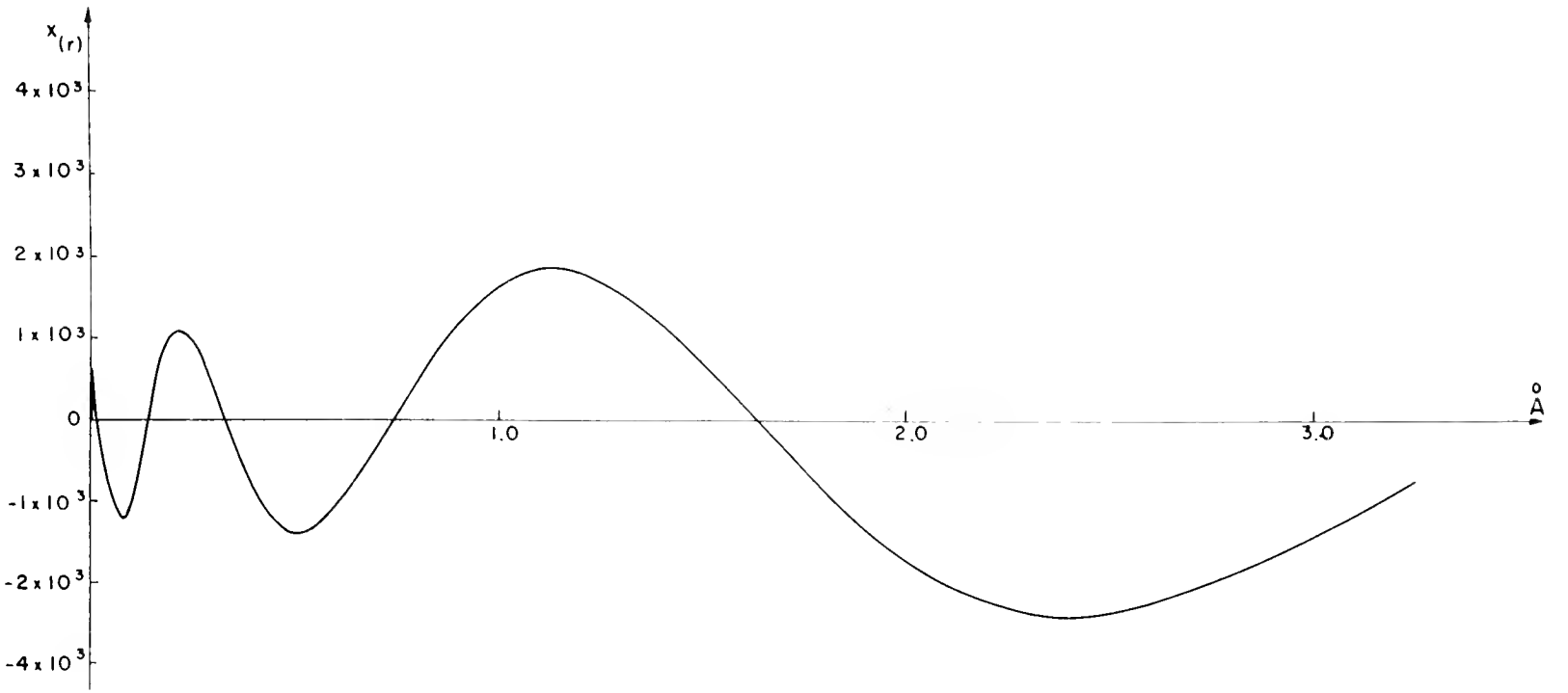


Cesium 7s State

$\varepsilon = 2.556439 \times 10^{-12}$

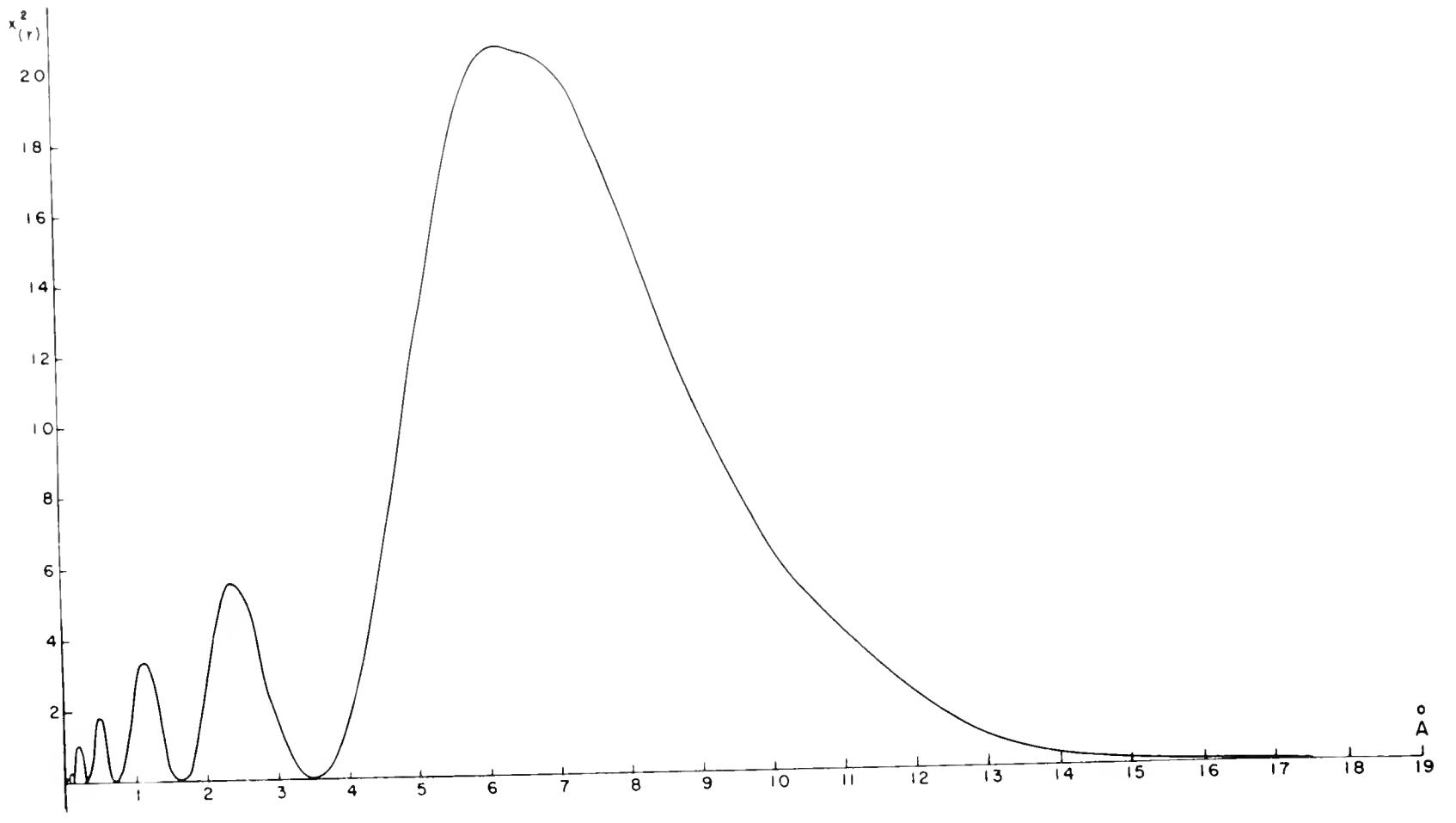
$\sigma_{r_o} = 7.07\ \%$

Figure 1



Inner Solution Expanded

Figure 2



Probability Distribution

Figure 3

EPSILON	RMAX	NORMALIZATION	ALPHA(RO)
2.556439E-12	2.450235E-07	8.246397E 00	7.070833E-02

INNER SOLUTION

R	CHI	CHISQ
2.357331E-11	1.515622E 02	2.297110E 04
1.023573E-09	-9.890845E 02	9.782882E 05
2.023573E-09	1.031266E 03	1.063510E 06
3.023573E-09	4.474262E 02	2.001902E 05
4.023573E-09	-8.278346E 02	6.853101E 05
5.023573E-09	-1.337223E 03	1.788165E 06
6.023573E-09	-1.038766E 03	1.079035E 06
7.023573E-09	-3.096236E 02	9.586680E 04
8.023573E-09	5.037750E 02	2.537892E 05
9.023573E-09	1.186158E 03	1.406972E 06
1.002357E-08	1.637021E 03	2.679838E 06
1.102357E-08	1.832169E 03	3.356843E 06
1.202357E-08	1.791166E 03	3.208274E 06
1.302357E-08	1.555250E 03	2.418804E 06
1.402357E-08	1.173848E 03	1.377919E 06
1.502357E-08	6.968905E 02	4.856564E 05
1.602357E-08	1.707055E 02	2.914035E 04
1.702357E-08	-3.640405E 02	1.325255E 05
1.802357E-08	-8.732911E 02	7.626373E 05
1.902357E-08	-1.329982E 03	1.768853E 06
2.002357E-08	-1.714144E 03	2.938290E 06
2.102357E-08	-2.012828E 03	4.051478E 06
2.202357E-08	-2.219864E 03	4.927795E 06
2.302357E-08	-2.335359E 03	5.453901E 06
2.402357E-08	-2.364870E 03	5.592611E 06
2.502357E-08	-2.318172E 03	5.373922E 06
2.602357E-08	-2.207670E 03	4.873806E 06
2.702357E-08	-2.046629E 03	4.188688E 06
2.802357E-08	-1.847520E 03	3.413331E 06
2.902357E-08	-1.620835E 03	2.627107E 06
3.002357E-08	-1.374587E 03	1.889489E 06
3.102357E-08	-1.114507E 03	1.242126E 06
3.202357E-08	-8.446624E 02	7.134545E 05

OUTER SOLUTION

R	CHI	CHISQ
3.242352E-08	-7.346993E 02	5.397830E 05
4.242352E-08	1.975877E 03	3.904092E 06
5.242352E-08	3.828054E 03	1.465400E 07
6.242352E-08	4.544958E 03	2.065664E 07
7.242352E-08	4.409886E 03	1.944709E 07
8.242352E-08	3.808746E 03	1.450655E 07
9.242352E-08	3.044773E 03	9.270641E 06
1.024235E-07	2.302172E 03	5.299995E 06
1.124235E-07	1.668634E 03	2.784339E 06
1.224235E-07	1.169875E 03	1.368607E 06
1.324235E-07	7.984085E 02	6.374561E 05
1.424235E-07	5.329000E 02	2.839824E 05
1.524235E-07	3.490897E 02	1.218636E 05
1.624235E-07	2.250614E 02	5.065263E 04
1.724235E-07	1.431219E 02	2.048388E 04
1.824235E-07	8.994511E 01	8.090123E 03
1.924235E-07	5.596465E 01	3.132042E 03
2.024235E-07	3.455357E 01	1.193949E 03
2.124235E-07	2.125141E 01	4.516222E 02
2.224235E-07	1.313141E 01	1.724340E 02
2.324235E-07	8.323815E 00	6.928589E 01
2.424235E-07	5.680861E 00	3.227218E 01

EPSILON	RMAX	NORMALIZATION	ALPHA(R0)
2.556439E-12	2.450235E-07	8.246397E 00	7.070833E-02

INNER SOLUTION

R	CHI	CHISQ
2.357331E-11	1.515622E 02	2.297110E 04
1.235733E-10	1.990095E 02	3.960477E 04
2.235733E-10	-1.011668E 02	1.023472E 04
3.235733E-10	-3.479303E 02	1.210555E 05
4.235733E-10	-5.931107E 02	3.517802E 05
5.235733E-10	-8.240385E 02	6.790394E 05
6.235733E-10	-1.019018E 03	1.038398E 06
7.235733E-10	-1.146263E 03	1.313918E 06
8.235733E-10	-1.184067E 03	1.402015E 06
9.235733E-10	-1.128031E 03	1.272455E 06
1.023573E-09	-9.890845E 02	9.782882E 05
1.123573E-09	-7.870408E 02	6.194332E 05
1.223573E-09	-5.444819E 02	2.964605E 05
1.323573E-09	-2.827089E 02	7.992432E 04
1.423573E-09	-1.973898E 01	3.896271E 02
1.523573E-09	2.303196E 02	5.304710E 04
1.623573E-09	4.571483E 02	2.089845E 05
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1.823573E-09	8.160009E 02	6.658575E 05
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2.323573E-09	1.095917E 03	1.201034E 06
2.423573E-09	1.058528E 03	1.120482E 06
2.523573E-09	9.970825E 02	9.941735E 05
2.623573E-09	9.150408E 02	8.372997E 05
2.723573E-09	8.158314E 02	6.655809E 05
2.823573E-09	7.027680E 02	4.938829E 05
2.923573E-09	5.789908E 02	3.352303E 05
3.023573E-09	4.474262E 02	2.001902E 05
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3.823573E-09	-6.154730E 02	3.788071E 05
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4.223573E-09	-1.004998E 03	1.010020E 06
4.323573E-09	-1.079541E 03	1.165408E 06
4.423573E-09	-1.144518E 03	1.309921E 06
4.523573E-09	-1.199900E 03	1.439759E 06
4.623572E-09	-1.245742E 03	1.551874E 06
4.723572E-09	-1.282176E 03	1.643976E 06
4.823572E-09	-1.309395E 03	1.714516E 06
4.923572E-09	-1.327646E 03	1.762645E 06
5.023572E-09	-1.337223E 03	1.788165E 06
5.123572E-09	-1.338454E 03	1.791459E 06
5.223572E-09	-1.331699E 03	1.773423E 06
5.323572E-09	-1.317342E 03	1.735390E 06

5.423572E-09	-1.295783E 03	1.679055E 06
5.523572E-09	-1.267437E 03	1.606397E 06
5.623572E-09	-1.232726E 03	1.519613E 06
5.723572E-09	-1.192076E 03	1.421045E 06
5.823572E-09	-1.145916E 03	1.313123E 06
5.923572E-09	-1.094672E 03	1.198307E 06
6.023572E-09	-1.038766E 03	1.079035E 06
6.123572E-09	-9.786137E 02	9.576848E 05
6.223572E-09	-9.146221E 02	8.365337E 05
6.323572E-09	-8.471888E 02	7.177289E 05
6.423572E-09	-7.767000E 02	6.032629E 05
6.523572E-09	-7.035300E 02	4.949545E 05
6.623572E-09	-6.280401E 02	3.944343E 05
6.723571E-09	-5.505779E 02	3.031361E 05
6.823571E-09	-4.714773E 02	2.222909E 05
6.923571E-09	-3.910576E 02	1.529261E 05
7.023571E-09	-3.096236E 02	9.586680E 04
7.123571E-09	-2.274656E 02	5.174059E 04
7.223571E-09	-1.448590E 02	2.098413E 04
7.323571E-09	-6.206492E 01	3.852054E 03
7.423571E-09	2.067004E 01	4.272504E 02
7.523571E-09	1.031134E 02	1.063237E 04
7.623571E-09	1.850466E 02	3.424224E 04
7.723571E-09	2.662646E 02	7.089686E 04
7.823571E-09	3.465759E 02	1.201148E 05
7.923571E-09	4.258014E 02	1.813069E 05
8.023571E-09	5.037750E 02	2.537892E 05
8.123570E-09	5.803423E 02	3.367972E 05
8.223570E-09	6.553609E 02	4.294979E 05
8.323570E-09	7.286993E 02	5.310027E 05
8.423570E-09	8.002372E 02	6.403796E 05
8.523570E-09	8.698643E 02	7.566640E 05
8.623570E-09	9.374806E 02	8.788699E 05
8.723570E-09	1.002995E 03	1.006000E 06
8.823570E-09	1.066327E 03	1.137054E 06
8.923570E-09	1.127403E 03	1.271038E 06
9.023569E-09	1.186158E 03	1.406972E 06
9.123569E-09	1.242537E 03	1.543897E 06
9.223569E-09	1.296488E 03	1.680882E 06
9.323569E-09	1.347972E 03	1.817027E 06
9.423569E-09	1.396951E 03	1.951472E 06
9.523569E-09	1.443397E 03	2.083396E 06
9.623569E-09	1.487288E 03	2.212024E 06
9.723569E-09	1.528605E 03	2.336632E 06
9.823569E-09	1.567336E 03	2.456543E 06
9.923569E-09	1.603476E 03	2.571135E 06
1.002357E-08	1.637021E 03	2.679838E 06
1.012357E-08	1.667974E 03	2.782139E 06
1.022357E-08	1.696342E 03	2.877577E 06
1.032357E-08	1.722135E 03	2.965748E 06
1.042357E-08	1.745366E 03	3.046304E 06
1.052357E-08	1.766055E 03	3.118949E 06
1.062357E-08	1.784220E 03	3.183441E 06
1.072357E-08	1.799886E 03	3.239591E 06
1.082357E-08	1.813080E 03	3.287260E 06
1.092357E-08	1.823831E 03	3.326358E 06
1.102357E-08	1.832169E 03	3.356843E 06
1.112357E-08	1.838129E 03	3.378717E 06
1.122357E-08	1.841746E 03	3.392028E 06
1.132357E-08	1.843058E 03	3.396861E 06
1.142357E-08	1.842103E 03	3.393345E 06
1.152357E-08	1.838924E 03	3.381640E 06

1.162357E-08	1.833561E 03	3.361946E 06
1.172357E-08	1.826059E 03	3.334490E 06
1.182357E-08	1.816461E 03	3.299532E 06
1.192357E-08	1.804815E 03	3.257357E 06
1.202357E-08	1.791166E 03	3.208274E 06
1.212357E-08	1.775561E 03	3.152617E 06
1.222357E-08	1.758049E 03	3.090738E 06
1.232357E-08	1.738680E 03	3.023007E 06
1.242357E-08	1.717501E 03	2.949809E 06
1.252357E-08	1.694563E 03	2.871543E 06
1.262357E-08	1.669916E 03	2.788618E 06
1.272357E-08	1.643610E 03	2.701454E 06
1.282357E-08	1.615697E 03	2.610476E 06
1.292357E-08	1.586227E 03	2.516115E 06
1.302357E-08	1.555250E 03	2.418804E 06
1.312357E-08	1.522819E 03	2.318978E 06
1.322357E-08	1.488984E 03	2.217074E 06
1.332357E-08	1.453796E 03	2.113524E 06
1.342357E-08	1.417306E 03	2.008757E 06
1.352356E-08	1.379565E 03	1.903200E 06
1.362356E-08	1.340623E 03	1.797270E 06
1.372356E-08	1.300530E 03	1.691379E 06
1.382356E-08	1.259337E 03	1.585930E 06
1.392356E-08	1.217093E 03	1.481316E 06
1.402356E-08	1.173848E 03	1.377919E 06
1.412356E-08	1.129651E 03	1.276110E 06
1.422356E-08	1.084549E 03	1.176247E 06
1.432356E-08	1.038592E 03	1.078674E 06
1.442356E-08	9.918276E 02	9.837220E 05
1.452356E-08	9.443025E 02	8.917072E 05
1.462356E-08	8.960637E 02	8.029302E 05
1.472356E-08	8.471576E 02	7.176760E 05
1.482356E-08	7.976300E 02	6.362136E 05
1.492356E-08	7.475260E 02	5.587952E 05
1.502356E-08	6.968905E 02	4.856564E 05
1.512356E-08	6.457675E 02	4.170156E 05
1.522356E-08	5.942005E 02	3.530742E 05
1.532356E-08	5.422325E 02	2.940161E 05
1.542356E-08	4.899058E 02	2.400077E 05
1.552356E-08	4.372622E 02	1.911982E 05
1.562356E-08	3.843427E 02	1.477193E 05
1.572356E-08	3.311878E 02	1.096854E 05
1.582356E-08	2.778373E 02	7.719356E 04
1.592356E-08	2.243303E 02	5.032410E 04
1.602356E-08	1.707055E 02	2.914035E 04
1.612356E-08	1.170005E 02	1.368911E 04
1.622356E-08	6.325258E 01	4.000888E 03
1.632356E-08	9.498233E 00	9.021642E 01
1.642356E-08	-4.422673E 01	1.956004E 03
1.652356E-08	-9.788719E 01	9.581901E 03
1.662356E-08	-1.514487E 02	2.293670E 04
1.672356E-08	-2.048775E 02	4.197478E 04
1.682356E-08	-2.581405E 02	6.663652E 04
1.692356E-08	-3.112054E 02	9.684880E 04
1.702356E-08	-3.640405E 02	1.325255E 05
1.712356E-08	-4.166149E 02	1.735680E 05
1.722356E-08	-4.688982E 02	2.198655E 05
1.732356E-08	-5.208610E 02	2.712962E 05
1.742356E-08	-5.724744E 02	3.277269E 05
1.752356E-08	-6.237102E 02	3.890145E 05
1.762356E-08	-6.745411E 02	4.550057E 05
1.772356E-08	-7.249403E 02	5.255384E 05

1.782356E-08	-7.748817E 02	6.004417E 05
1.792356E-08	-8.243402E 02	6.795368E 05
1.802356E-08	-8.732911E 02	7.626373E 05
1.812356E-08	-9.217105E 02	8.495502E 05
1.822356E-08	-9.695752E 02	9.400761E 05
1.832356E-08	-1.016863E 03	1.034010E 06
1.842356E-08	-1.063552E 03	1.131142E 06
1.852356E-08	-1.109621E 03	1.231258E 06
1.862356E-08	-1.155050E 03	1.334140E 06
1.872356E-08	-1.199819E 03	1.439565E 06
1.882356E-08	-1.243909E 03	1.547310E 06
1.892355E-08	-1.287303E 03	1.657149E 06
1.902355E-08	-1.329982E 03	1.768853E 06
1.912355E-08	-1.371930E 03	1.882193E 06
1.922355E-08	-1.413131E 03	1.996940E 06
1.932355E-08	-1.453570E 03	2.112865E 06
1.942355E-08	-1.493231E 03	2.229739E 06
1.952355E-08	-1.532101E 03	2.347334E 06
1.962355E-08	-1.570167E 03	2.465424E 06
1.972355E-08	-1.607415E 03	2.583785E 06
1.982355E-08	-1.643835E 03	2.702194E 06
1.992355E-08	-1.679415E 03	2.820434E 06
2.002355E-08	-1.714144E 03	2.938290E 06
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2.022355E-08	-1.781012E 03	3.172003E 06
2.032355E-08	-1.813133E 03	3.287452E 06
2.042355E-08	-1.844369E 03	3.401695E 06
2.052355E-08	-1.874711E 03	3.514542E 06
2.062355E-08	-1.904154E 03	3.625804E 06
2.072355E-08	-1.932693E 03	3.735300E 06
2.082355E-08	-1.960320E 03	3.842856E 06
2.092355E-08	-1.987034E 03	3.948303E 06
2.102355E-08	-2.012828E 03	4.051478E 06
2.112355E-08	-2.037701E 03	4.152227E 06
2.122355E-08	-2.061650E 03	4.250402E 06
2.132355E-08	-2.084673E 03	4.345860E 06
2.142355E-08	-2.106768E 03	4.438470E 06
2.152355E-08	-2.127935E 03	4.528106E 06
2.162355E-08	-2.148173E 03	4.614648E 06
2.172355E-08	-2.167484E 03	4.697987E 06
2.182355E-08	-2.185868E 03	4.778020E 06
2.192355E-08	-2.203327E 03	4.854651E 06
2.202355E-08	-2.219864E 03	4.927795E 06
2.212355E-08	-2.235480E 03	4.997372E 06
2.222355E-08	-2.250180E 03	5.063310E 06
2.232355E-08	-2.263967E 03	5.125548E 06
2.242355E-08	-2.276846E 03	5.184029E 06
2.252355E-08	-2.288822E 03	5.238706E 06
2.262355E-08	-2.299900E 03	5.289539E 06
2.272355E-08	-2.310086E 03	5.336496E 06
2.282355E-08	-2.319386E 03	5.379552E 06
2.292355E-08	-2.327808E 03	5.418691E 06
2.302355E-08	-2.335359E 03	5.453901E 06
2.312355E-08	-2.342046E 03	5.485181E 06
2.322355E-08	-2.347879E 03	5.512534E 06
2.332355E-08	-2.352865E 03	5.535971E 06
2.342355E-08	-2.357013E 03	5.555510E 06
2.352354E-08	-2.360333E 03	5.571173E 06
2.362354E-08	-2.362835E 03	5.582992E 06
2.372354E-08	-2.364530E 03	5.591000E 06
2.382354E-08	-2.365426E 03	5.595241E 06
2.392354E-08	-2.365536E 03	5.595761E 06

2.402354E-08	-2.364870E 03	5.592611E 06
2.412354E-08	-2.363440E 03	5.585848E 06
2.422354E-08	-2.361257E 03	5.575535E 06
2.432354E-08	-2.358334E 03	5.561737E 06
2.442354E-08	-2.354681E 03	5.544525E 06
2.452354E-08	-2.350313E 03	5.523972E 06
2.462354E-08	-2.345241E 03	5.500155E 06
2.472354E-08	-2.339478E 03	5.473157E 06
2.482354E-08	-2.333037E 03	5.443060E 06
2.492354E-08	-2.325930E 03	5.409952E 06
2.502354E-08	-2.318172E 03	5.373922E 06
2.512354E-08	-2.309775E 03	5.335061E 06
2.522354E-08	-2.300753E 03	5.293463E 06
2.532354E-08	-2.291118E 03	5.249222E 06
2.542354E-08	-2.280885E 03	5.202437E 06
2.552354E-08	-2.270067E 03	5.153203E 06
2.562354E-08	-2.258677E 03	5.101621E 06
2.572354E-08	-2.246729E 03	5.047790E 06
2.582354E-08	-2.234236E 03	4.991811E 06
2.592354E-08	-2.221212E 03	4.933783E 06
2.602354E-08	-2.207670E 03	4.873806E 06
2.612354E-08	-2.193623E 03	4.811982E 06
2.622354E-08	-2.179085E 03	4.748411E 06
2.632354E-08	-2.164068E 03	4.683191E 06
2.642354E-08	-2.148586E 03	4.616423E 06
2.652354E-08	-2.132652E 03	4.548202E 06
2.662354E-08	-2.116277E 03	4.478628E 06
2.672354E-08	-2.099475E 03	4.407796E 06
2.682354E-08	-2.082258E 03	4.335800E 06
2.692354E-08	-2.064639E 03	4.262733E 06
2.702354E-08	-2.046629E 03	4.188688E 06
2.712354E-08	-2.028239E 03	4.113754E 06
2.722354E-08	-2.009483E 03	4.038020E 06
2.732354E-08	-1.990370E 03	3.961573E 06
2.742354E-08	-1.970913E 03	3.884496E 06
2.752354E-08	-1.951121E 03	3.806874E 06
2.762354E-08	-1.931007E 03	3.728786E 06
2.772354E-08	-1.910579E 03	3.650313E 06
2.782354E-08	-1.889849E 03	3.571529E 06
2.792354E-08	-1.868826E 03	3.492511E 06
2.802354E-08	-1.847520E 03	3.413331E 06
2.812354E-08	-1.825941E 03	3.334060E 06
2.822353E-08	-1.804097E 03	3.254765E 06
2.832353E-08	-1.781997E 03	3.175514E 06
2.842353E-08	-1.759650E 03	3.096370E 06
2.852353E-08	-1.737065E 03	3.017396E 06
2.862353E-08	-1.714250E 03	2.938652E 06
2.872353E-08	-1.691211E 03	2.860195E 06
2.882353E-08	-1.667958E 03	2.782083E 06
2.892353E-08	-1.644497E 03	2.704370E 06
2.902353E-08	-1.620835E 03	2.627107E 06
2.912353E-08	-1.596980E 03	2.550345E 06
2.922353E-08	-1.572937E 03	2.474132E 06
2.932353E-08	-1.548714E 03	2.398516E 06
2.942353E-08	-1.524317E 03	2.323542E 06
2.952353E-08	-1.499751E 03	2.249252E 06
2.962353E-08	-1.475022E 03	2.175690E 06
2.972353E-08	-1.450136E 03	2.102894E 06
2.982353E-08	-1.425098E 03	2.030904E 06
2.992353E-08	-1.399913E 03	1.959757E 06
3.002353E-08	-1.374587E 03	1.889489E 06
3.012353E-08	-1.349124E 03	1.820135E 06

3.022353E-08	-1.323528E 03	1.751726E 06
3.032353E-08	-1.297805E 03	1.684297E 06
3.042353E-08	-1.271958E 03	1.617876E 06
3.052353E-08	-1.245991E 03	1.552494E 06
3.062353E-08	-1.219910E 03	1.488180E 06
3.072353E-08	-1.193717E 03	1.424960E 06
3.082353E-08	-1.167416E 03	1.362861E 06
3.092353E-08	-1.141012E 03	1.301908E 06
3.102353E-08	-1.114507E 03	1.242126E 06
3.112353E-08	-1.087906E 03	1.183539E 06
3.122353E-08	-1.061211E 03	1.126168E 06
3.132353E-08	-1.034425E 03	1.070036E 06
3.142352E-08	-1.007553E 03	1.015163E 06
3.152352E-08	-9.805970E 02	9.615704E 05
3.162352E-08	-9.535600E 02	9.092766E 05
3.172352E-08	-9.264451E 02	8.583006E 05
3.182352E-08	-8.992554E 02	8.086602E 05
3.192352E-08	-8.719935E 02	7.603727E 05
3.202352E-08	-8.446624E 02	7.134545E 05
3.212352E-08	-8.172647E 02	6.679216E 05
3.222352E-08	-7.898032E 02	6.237891E 05
3.232352E-08	-7.622805E 02	5.810716E 05
3.242352E-08	-7.346993E 02	5.397830E 05

OUTER SOLUTION

R	CHI	CHISQ
3.242352E-08	-7.346993E 02	5.397830E 05
3.342352E-08	-4.562168E 02	2.081338E 05
3.442352E-08	-1.745197E 02	3.045714E 04
3.542352E-08	1.082300E 02	1.171374E 04
3.642352E-08	3.900763E 02	1.521595E 05
3.742352E-08	6.692551E 02	4.479024E 05
3.842352E-08	9.441875E 02	8.914900E 05
3.942352E-08	1.213471E 03	1.472512E 06
4.042352E-08	1.475872E 03	2.178199E 06
4.142352E-08	1.730316E 03	2.993993E 06
4.242352E-08	1.975877E 03	3.904092E 06
4.342352E-08	2.211772E 03	4.891937E 06
4.442352E-08	2.437348E 03	5.940665E 06
4.542352E-08	2.652072E 03	7.033487E 06
4.642352E-08	2.855526E 03	8.154031E 06
4.742351E-08	3.047394E 03	9.286611E 06
4.842351E-08	3.227455E 03	1.041646E 07
4.942351E-08	3.395574E 03	1.152992E 07
5.042351E-08	3.551693E 03	1.261453E 07
5.142351E-08	3.695828E 03	1.365914E 07
5.242351E-08	3.828054E 03	1.465400E 07
5.342351E-08	3.948506E 03	1.559070E 07
5.442351E-08	4.057365E 03	1.646221E 07
5.542351E-08	4.154860E 03	1.726286E 07
5.642351E-08	4.241255E 03	1.798825E 07
5.742351E-08	4.316850E 03	1.863520E 07
5.842351E-08	4.381971E 03	1.920167E 07
5.942351E-08	4.436967E 03	1.968667E 07
6.042351E-08	4.482205E 03	2.009016E 07
6.142351E-08	4.518070E 03	2.041296E 07
6.242351E-08	4.544958E 03	2.065664E 07
6.342351E-08	4.563272E 03	2.082345E 07
6.442351E-08	4.573422E 03	2.091619E 07
6.542351E-08	4.575820E 03	2.093813E 07
6.642350E-08	4.570880E 03	2.089294E 07
6.742350E-08	4.559014E 03	2.078461E 07
6.842350E-08	4.540631E 03	2.061733E 07
6.942350E-08	4.516133E 03	2.039546E 07
7.042350E-08	4.485918E 03	2.012346E 07
7.142350E-08	4.450375E 03	1.980584E 07
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